# Continuum Dynamics (CCS-2) Publications and Presentations, March 2004-March 2005

### **Telluride Team**

- B. Cooke, B. Smith, et al., "Modeling the MTI Electro-Optic System Sensitivity and Resolution," IEEE Transactions on Geoscience and Remote Sensing, in press.
- J. Cullum, M. Hall, W. Joubert, T. Betlach, and B. Lally, "Scalable Parallel Linear Solvers for ASCI Applications—Scaling Across Thousands of Processors," technical report LA-UR-04-1879, Los Alamos National Laboratory. (Presentation to the CCS Division Review Committee.)
- S. Cummins, M. Francois, D. Kothe, "Estimating Curvature from Volume Fractions, Computers and Structures," Vol. 83, Issue: 6-7, pp. 425-434, February 2005.
- S. Cummins and D. Kothe, "A Study of Eulerian Phase Front Models for Crystal Growth," technical report, LA-UR-04-2390, Los Alamos National Laboratory.
- S. Cummins, J. Mohd-Yusof, M. Francois, D. Kothe, "Eulerian Techniques for Crystal Growth," Telluride Workshop presentation, June 2004, and technical report, LA-UR-04-4250, Los Alamos National Laboratory.
- A. Davis, M. Hall, and Igor N. Polonsky, "Three-Dimensional Radiative Transfer, Simplified ... with Cloud Modeling and Remote Sensing in Mind," technical report, LA-UR-05-2282, Los Alamos National Laboratory. (Presentation to the ARM Science Team Meeting in Daytona Beach, Fla.)
- M. Francois, "Interfacial Flow Computations with the Volume of Fluid and Immersed Boundary Methods," presented at invited seminars at New Mexico State University, Texas A&M, and the University of Illinois at Urbana-Champaign. (Also a technical report, LA-UR-04-1852, Los Alamos National Laboratory.)
- M. Francois, "Modeling of Surface Tension Force within a Volume-of-Fluid Formulation," presented at a Los Alamos National Laboratory, CCS-2 seminar, June 2004. (Also a technical report, LA-UR-04-4207, Los Alamos National Laboratory.)
- M. Francois, S. Cummins, E. Dendy, D. Kothe, J. Sicilian, and M. Williams, "A Balanced-Force Algorithm for Continuous and Sharp Interfacial Surface Tension Models within a Volume Tracking Framework," technical report, LA-UR-05-0674, Los Alamos National Laboratory. (Also submitted to *Journal of Computational Physics*, 2005.)

- M. Francois, E. Dendy, D. Kothe, J. Sicilian, M. Williams, and S. Cummins, "Improvements on the Modeling of Surface Tension in Truchas," presented at the Truchas Workshop, Los Alamos, June 2004. (Also a technical paper, LA-UR-04-4103, Los Alamos National Laboratory.)
- M. Francois, D. Kothe, S. Cummins, "Modeling Surface Tension Using a Ghost Fluid Technique within a Volume of Fluid Formulation," in the Proceedings of the 21st International Congress on Theoretical and Applied Mechanics (ICTAM 04), Warsaw, Poland, August 2004. (Also a technical report, LA-UR-04-0413, Los Alamos National Laboratory.)
- M. Hall and A. Davis, "Progress Toward Higher-Fidelity Yet Efficient Modeling of Radiation Energy Transport through Three-Dimensional Clouds," technical report, LA-UR-05-2275, Los Alamos National Laboratory. (Also a presentation to the ARM Science Team Meeting in Daytona Beach, Fla.)
- W. Joubert, M. Hall, J. Cullum, T. Betlach, and Bryan Lally, "Experiences with Linear Solvers on ASCI Applications: Achieving Scalability and Related Issues," technical report, LA-UR-04-1462, Los Alamos National Laboratory. (Also a presentation to the ASCI Computational Physics Methods Workshop in Monterey, Calif.)
- W. Joubert, M. Hall, J. Cullum, and B. Lally, "The LAMG Solver Library: Recent Results and Future Plans," technical report, LA-UR-05-1345, Los Alamos National Laboratory. (Also a presentation at LANL.)
- D. Lorstad, M. Francois, W. Shyy, and L. Fuchs, "Assessment of Volume of Fluid and Immersed Boundary Methods for Droplet Computations," *International Journal for Numerical Methods in Fluids*, Vol. 46, pp. 109-125, September 2004.
- J. Turner, "Linear and Nonlinear Solvers in Truchas," technical report, LA-UR-04-4260, Los Alamos National Laboratory. (Also a presentation in June 2004 at the Second Annual Telluride Workshop.)
- J. Turner and D. Kothe, "Implications of Petascale Computing for LANL Applications," technical report, LA-UR number pending, Los Alamos National Laboratory. (Also a presentation in March 2005 at the Department of Energy Office of Science Petascale/s Compact Simulation Application Workshop.)
- J. Turner and S. Swaminarayan. "Radiative Heat Transfer in Truchas," technical report, LA-UR-04- 4329, Los Alamos National Laboratory. (Also a presentation in June 2004 at the Second Annual Telluride Workshop.)

### **Radiation Hydrodynamics Team**

M. Christon, "Compatible Extensions for Finite Element Lagrangian Hydrodynamics," to be presented at the Eighth U.S. National Congress on Computational Mechanics, Austin,

- Texas, July 24-28, 2005. (Also a technical report, LA-UR-05-2032, Los Alamos National Laboratory.)
- M. Christon and R. Patil, "A Finite Element Projection Method for Low-Mach Number Reacting Flows," to appear in Proceedings of the Third MIT Conference on Computational Fluid and Solid Mechanics, K.J. Bathe (editor), Elsevier, 2005. (Also a technical report, LA-UR-05-2031, Los Alamos National Laboratory.)
- G. Dilts, "Consistent Thermodynamic Derivative Estimates for Tabular Equations of State," submitted to *Physical Review E*, March 2005.
- G. Dilts, "Physically Realistic EOS Derivative Estimates," in the Proceedings of the Nuclear Explosives Code Developers Conference, Oct 4-7, 2004, Livermore, Calif.
- D. Holm, C. Jeffery, S. Kurien, D. Livescu, M. Taylor, and B. Wingate, "The LANS-Alpha Model for Computing Turbulence: Origins, Results, and Open Problems," *Los Alamos Science* 29, 152-171, 2005.
- K. Lipnikov, J. Morel, and M. Shashkov, "Mimetic Finite Difference Methods for Diffusion Equations on Non-Orthogonal Non-Conformal Meshes," *Journal of Computational Physics*, 199, 589-597, 2004.
- D. Livescu, "Characteristics of Small Scale Turbulence in Homogeneous Turbulent Shear Flow," 57th annual Meeting of the American Physical Society, Division of Fluid Dynamics, Seattle, Wash., November 23, 2004.
- D. Livescu, "Comment on Compressible Rayleigh-Taylor Instabilities in Supernova Remnants (*Phys. of Fluids* 16, 4661, [2004])," to appear in *Physics of Fluids*, 2005.
- D. Livescu, "Compressibility Effects on the Rayleigh-Taylor Instability," Turbulent Working Group Seminar, Los Alamos National Laboratory, July 7, 2004.
- D. Livescu, "Compressibility Effects on the Rayleigh-Taylor Instability in the Linear and Weakly Nonlinear Stage," Turbulent Mixing Group Colloquium, Los Alamos National Laboratory, June 28, 2004.
- D. Livescu, "Overview of the Compressible Rayleigh-Taylor Instability," LDRD-DR Seminar, Los Alamos National Laboratory, December 10, 2004.
- D. Livescu, "Stochastic Large Eddy Simulations on Coarse Grids," LDRD-DR review, Los Alamos National Laboratory, March 22, 2004.
- D. Livescu and C. Madnia, "Characteristics of Small Scale Turbulence in Homogeneous Turbulent Shear Flow," *Bulletin of American Physical Society* 49(10), 157, 2004. (Also presented at the 57th annual Meeting of the American Physical Society, Division of Fluid Dynamics, Seattle, Wash., November 21-23, 2004.)

- D. Livescu and C. Madnia, "Small Scale Structure of Homogeneous Turbulent Shear Flow," *Physics of Fluids* 16(8), 2864-2876, 2004.
- R. Loubere and E. Caramana, "The Force/Work Differencing of Exceptional Points in the Discrete, Compatible Formulation of Lagrangian Hydrodynamics," technical report, LAUR-04-8906, Los Alamos National Laboratory.
- J. Morel, B. Adams, Taewan Noh, J. McGhee, T. Evans, and T. Urbatsch, "Spatial Discretizations for Self-Adjoint Forms of the Radiative Transfer Equations," submitted to the *Journal of Computational Physics*.
- J. Morel and J. Densmore, "A Two-Component Equilibrium Diffusion Limit," *Annals of Nuclear Energy*, 31, 2049-2057, 2004.
- J. Morel and K. Lathrop, "Singular Solutions, Integral Transport Theory, and the Sn Method," *Nuclear Science and Engineering*, 147, 158-166, 2004.
- J. Morel and J. Warsa, "An Sn Spatial Discretization Scheme for Tetrahedral Meshes," to appear in *Nuclear Science and Engineering*.
- J. Morel and J. Warsa, "Sn Finite-Element Lumping on Quadrilateral Meshes in \$X-Y\$ Geometry," accepted for presentation, MC2005:International Topical Meeting on Mathematics and Computation, Supercomputing, Reactor Physics, and Nuclear and Biological Applications, Avignon, France, September 12-15, 2005.
- B. Nadiga, D. Livescu, and C. McKay, "Stochastic Large Eddy Simulations of Geostrophic Turbulence," to be presented at the 2005 General Assembly meeting of the European Geophysical Union, Vienna, Austria, April 2005.
- B. Nadiga, D. Livescu, and C. McKay, "Stochastic Large Eddy Simulations of Geostrophic Turbulence," to be presented at the 2005 Joint Assembly meeting of the American Geophysical Union, New Orleans, May 2005.
- J. Ristorcelli and D. Livescu, "Decay of Isotropic Turbulence: A Tale of Two Decays," Cascade Dynamics: Fundamentals and Modeling Workshop, Santa Fe, N.M., August 16-19, 2004.
- J. Ristorcelli and D. Livescu, "Decay of Isotropic Turbulence: Fixed Points and Solutions for Non-Constant G R Palinstrophy," *Physics of Fluids*, 16(9), 3487-3490, 2004.
- J. Ristorcelli and D. Livescu, "Decay of Isotropic Turbulence: Fixed Points and Solutions for Non-Constant Palinstrophy," *Bulletin of American Physical Society*, 49(10), 112, 2004. (Also presented at the 57th annual Meeting of the American Physical Society, Division of Fluid Dynamics, Seattle, Wash., November 21-23, 2004.)

- M. Rosa, Y. Azmy, and J. Morel, "Properties of the Sn-Equivalent Integral Transport Operator in Heterogeneous Slabs," accepted for presentation, MC2005:International Topical Meeting on Mathematics and Computation, Supercomputing, Reactor Physics, and Nuclear and Biological Applications, Avignon, France, September 12-15, 2005.
- M. Rosa, Y. Azmy, and J. Morel, "Properties of the Sn-Equivalent Integral Transport Operator in Slab Geometry," accepted for presentation at the American Nuclear Society Annual Meeting, San Diego, Calif., June 5-9, 2005.
- R. Rubinstein, T. Clark, D. Livescu, and L. Luo, "Time-Dependent Isotropic Turbulence," *Journal of Turbulence* 5, 011, 1-16, 2004.
- R. Ward, R. Baker, and J. Morel, "A Diffusion Synthetic Acceleration Method for Block Adaptive Mesh Refinement," submitted to *Nuclear Science and Engineering*.
- J. Warsa, M. Benzi, T. Wareing, and J. Morel, "Preconditioning a Mixed Discontinuous Finite Element Method for Radiation Diffusion," to appear in *Journal on Numerical Linear Algebra with Applications*.
- J. Warsa, T. Wareing, and J. Morel, "Krylov Iterative Methods and the Degraded Effectiveness of Diffusion Synthetic Acceleration for Multidimensional Sn Calculations in Problems with Material Discontinuities," *Nuclear Science and Engineering*, 147, 218-248, 2004.
- J. Warsa, T. Wareing, J. Morel, J. McGhee, and R. Lehoucq, "Krylov Subspace Iterations for Deterministic k-Eigenvalue Calculations," *Nuclear Science and Engineering*, 147, 26-42 (2004).

# **Climate and Ocean Modeling Team**

- S. Belviso, S. Elliott, et al, "Comparison of Global Climatological Maps of Sea Surface Dimethylsulfide," *Global Biogeochemical Cycles*, 18: 10.1029/2003GB002193.
- R. Bleck, M. Maltrud, S. Chu, F. Chai, F. Chavez, and S. Elliott, "Comparison of Cartesian and Isopycnal Simulations of Oceanic Carbon Sequestration via Iron Fertilization and Deep Injection," University of Miami web page.
- C. Cao, D. Holm, and E. Titi, "Traveling Wave Solutions for a Class of One-Dimensional Nonlinear Shallow Water Wave Models," *J. of Dyn. and Diff. Eqns.*, 16, 167-178, 2004.
- S. Chu, S. Elliott, M. Maltrud, and F. Chai, "Iron Patch Enrichments in the Southern Ocean of a Global Eddy Permitting General Circulation Model," in *ESEC*, Vol. 2, FiatLux: Chapter 8.

- S. Chu, S. Elliott, M. Maltrud, and D. Erickson, "Ecodynamic and Eddy Admitting Simulations of Dimethyl Sulfide Distributions in the Parallel Ocean Program," *Earth Interactions*, 8: 1-25.
- R. Cushman, H. Dullin, A. Giacobbe, D. Holm, M. Joyeux, P. Lynch, D. Sadovskii, and B. Zhilinskii, "The CO2 Molecule as a Quantum Realization of the 1:1:2 Resonant Swing-Spring with Monodromy," *Phys. Rev. Lett.* 93, 024302-5, 2004. (This four-page paper received a two-page review in Ian Stewart, *Nature* 430, 731-732, 2004.)
- H. Dullin, G. Gottwald, and D. Holm, "On Asymptotically Equivalent Shallow Water Wave Equations," *Physica D* 190, 1-14, 2004.
- S. Elliott and S. Chu, "Algorithms for Analytical Optimization of Large Scale Marine Trace Gas Cycling Constants," technical report, LA-UR-05-2044, Los Alamos National Laboratory.
- S. Elliott, S. Chu, and D. Erickson, "Contours of Simulated Marine Dimethyl Sulfide Distributions under Variation in a Gabric Mechanism," technical report, technical report, LA-UR-05-1582, Los Alamos National Laboratory.
- S. Elliott, S. Chu, M. Maltrud, and A. McPherson, "Animation of Global Marine Chlorophyll Distributions from Fine Grid Biogeochemistry/Transport Modeling," in *ESEC*, Vol. 2, FiatLux: Chapter 9.
- S. Elliott, M. Maltrud, S. Chu, and D. Erickson, "A Marine Trace Gas Cycling Module for Community Climate System Simulations," technical report, LA-UR-04-8200, Los Alamos National Laboratory.
- S. Elliott, M. Maltrud, S. Chu, and D. Erickson, "TRACEGAS\_MOD: Processing for Low Concentration Volatiles in the Community Climate System Model Ocean," submitted to *Environmental Modeling and Software*. (Also a technical report, LA-UR-05-0673, Los Alamos National Laboratory.)
- P. Gent, F. Bryan, G. Danabasoglu, K. Lindsay, D. Tsumune, M. Hecht, S. Doney, "Ocean Chlorofluorocarbon and Heat Uptake During the 20th Century in the CCSM3," submitted to the *Journal of Climate*. (Also a technical report, LA-UR-05-0888, Los Alamos National Laboratory.)
- B. Geurts and D. Holm, "Nonlinear Regularization for Large-Eddy Simulation in Direct and Large-Eddy Simulation V," in Proceedings of DLES5, Munich, August 27-29, 2003, R. Friedrich, B. J. Geurts, and O. Metais (editors), Kluwer Academic Publishers, pp 5-14, 2004.
- M. Hecht, review (written at the request of the American Meteorological Society) of S. Griffies' book, "Fundamentals of Ocean Climate Models," Princeton University Press. Review to appear in the *Bulletin of the American Meteorological Society*.

- D. Holm, "The Euler-Poincare Variational Framework for Modeling Fluid Dynamics," in Geometric Mechanics and Symmetry: The Peyresq Lectures, J. Montaldi and T. Ratiu (editors), London Mathematical Society Lecture Notes Series 306, Cambridge University Press, 2005.
- D. Holm, "Taylor's Hypothesis, Hamilton's Principle, and the LANS-Alpha Model for Computing Turbulence," Science-Based Prediction for Complex Systems, N. Cooper (editor), *Los Alamos Science* 29, 172-180, 2005.
- D. Holm and B. Fabijonas, "Craik-Criminale Solutions and Elliptic Instability in Nonlinear-Reactive Closure Models for Turbulence," *Phys. Fluids* 16, 853-866, 2004.
- D. Holm and B. Fabijonas, "Euler-Poincare Formulation and Elliptic Instability for Nth-Gradient Fluids," *J. Phys. A: Math. Gen.* 37, 7609-7623, 2004.
- D. Holm and B. Fabijonas, "Multi-Frequency Craik-Criminale Solutions of the Navier-Stokes Equations," *J. Fluid Mech.* 506, 207-215, 2004.
- D. Holm and A. Hone, "A Class of Equations with Peakon and Pulson Solutions," (with an appendix by H. Braden and J. Byatt-Smith, *D. D. J. of Nonlin. Math. Phys.* 12, Supplement 1, 1-15, 2005.
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- D. Holm and J. Marsden, "Momentum Maps and Measure Valued Solutions (Peakons, Filaments, and Sheets) of the Euler-Poincare Equations for the Diffeomorphism Group," in The Breadth of Symplectic and Poisson Geometry, a Festshrift, for A. Weinstein, J. Marsden, and T. Ratiu (editors), Birkhauser Boston, *Progr. Math.* 232, 203-235, 2004.
- D. Holm, V. Putkaradze, and S. Stechmann, "Rotating Concentric Circular Peakons," *Nonlinearity* 17, 1-24, 2004.
- D. Holm, J. Rananather, A. Trouve, and L. Younes, "Soliton Dynamics in Computational Anatomy," *NeuroImage* 23, S170-178, 2004.
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- B. Nadiga, "Proposal for Organizing 'Stochastic Closure for Large Scale Turbulent Flows," accepted for AGU Joint Assembly, New Orleans, 2005.

- B. Nadiga, "Proposal for Organizing 'Stochastic Dynamics," accepted for EGU, Vienna, Austria, 2005.
- B. Nadiga and D. Straub, "Organized 'Dynamics of Ocean Circulation," AGU Joint Assembly, Montreal, Canada, May 2004.
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- M. Petersen, B. Kraus, and T. Windham, "Striving Towards Equity; Underrepresented Minorities and Mathematics," SIAM News, March (Part I), April (Part II).
- M. Taylor, B. Wingate, L. Bos, "A New Algorithm for Computing Multivariate Quadrature Points," submitted to the *SIAM Journal on Numerical Analysis*, 2004.
- B. Wingate, "The Maximum Allowable Time Step for the Shallow Water Alpha-Model and Its Relation to Time-Implicit Differencing," *Monthly Weather Review*, Vol. 132, pp. 2719, 2004.

## Hydro Methods for Thermonuclear Applications Team

- M. Christie, J. Glimm, J. Grove, D. Higdon, D. Sharp, and M. Wood-Schultz, "Error Analysis and Simulations of Complex Phenomena," *Los Alamos Science*, 29:2-25, 2005.
- E. Dendy, "Interface Models and Hydrodynamic Coupling for the Crestone Project (U)," limited-distribution report, LA-CP-05-0308, Los Alamos National Laboratory.
- E. Dendy, "The RAGE Hydrodynamics Algorithm," a technical report, LA-UR-05-1642, Los Alamos National Laboratory.
- S. Dutta, E. George, J. Glimm, J. Grove, H. Jin, T. Lee, X. Li, D. Sharp, K. Ye, Y. Yu, Y. Zhang, and M. Zhao, "Shock Wave Interactions in Spherical and Perturbed Spherical Geometries," Nonlinear Analysis, 2004. (In press: University at Stony Brook preprint number SB-AMS-04-09. Also, a technical report, LA-UR-04-2989, Los Alamos National Laboratory.)
- S. Dutta, J. Glimm, J. Grove, D. Sharp, and Y. Zhang, "Error Comparison in Tracked and Untracked Spherical Simulations," *Computers and Mathematics with Applications*, 48:1733-1747, 2004. (University at Stony Brook preprint number AMS-03-10. Also, a technical report, LA-UR-03-2920, Los Alamos National Laboratory.)
- S. Dutta, J. Glimm, J. Grove, D. Sharp, and Y. Zhang, "Spherical Richtmyer-Meshkov Instability for Axisymmetric Flow," Mathematics and Computers in Simulations, 65:417-430, 2004. (University at Stony Brook preprint number AMS-03-13.)

- J. Glimm, J. Grove, Y. Kang, T. Lee, X. Li, D. Sharp, Y. Yu, K. Ye, and M. Zhao, "Errors in Numerical Solutions of Spherically Symmetric Shock Physics Problems," *Contemporary Mathematics*, 371:163-179, 2005. (University at Stony Brook preprint number SB-AMS-04-03. Also, a technical report, LA-UR-04-0713, Los Alamos National Laboratory.)
- J. Glimm, J. Grove, Y. Kang, T. Lee, X. Li, D. Sharp, Y. Yu, K. Ye, and M. Zhao, "Statistical Riemann Problems and a Composition Law for Errors in Numerical Solutions of Shock Physics Problems," *SISC*, 26:666-697, 2004. (University at Stony Brook preprint number SB-AMS-03-11. Also, a technical report, LA-UR-03-2921, Los Alamos National Laboratory.)
- X. Li, J. Wohlbier, S. Jin, and J. Booske, "Eulerian Method for Computing Multi-valued Solutions of the Euler-Poisson Equations and Applications to Wave Breaking in Klystrons, *Phys. Rev. E* 70, 016502, 2004.
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- J. Wohlbier, S. Jin, and S. Sengele, "Eulerian Calculations of Wave Breaking and Multivalued Solutions in a Traveling Wave Tube," *Physics of Plasmas* 12, 023106, 2005.
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# **Data-Driven Modeling Team**

## LANL Reports

K. Borozdin, et al., "Information Extraction from Muon Radiography

- Data," technical report, LA-UR-04-3985. Los Alamos National Laboratory.
- T. Asaki, "Clustering and Likelihood Based Analysis for Muon Radiography," technical report, LA-UR-05-2659, Los Alamos National Laboratory.
- T. Asaki, "Elasticity Based TSWarp Cost Functions," technical report, LA-UR-04-4099, Los Alamos National Laboratory.
- T. Asaki, "The Geometry of a Beta-Layered Solid Grown on a Perturbed Boundary," technical report, LA-UR-04-4101, Los Alamos National Laboratory.
- T. Asaki, "Inverse Abel Transform Regularization," technical report, LA-UR-04-4100, Los Alamos National Laboratory.
- T. Asaki and K. Vixie, "SVD Analysis for Radiographic Object Reconstruction III: Total Variation Regularization," technical report, LA-UR-04-7076, Los Alamos National Laboratory.
- K. Vixie and T. Asaki, "Defensible Metrics and Merit Functions: Making Informative Comparisons of Computer Simulations and Experiments," technical report, LA-UR-04-8498, Los Alamos National Laboratory. (Also, an LDRD Progress Report in LA-05-0001-PR.)

### Journal Papers

- T. Asaki, P. Campbell, R. Chartrand, C. Powell, K. Vixie, and B. Wohlberg, "Abel Inversion Using Total Variation Regularization: Applications," submitted to *Inverse Problems in Science and Engineering*. (Also, a technical report, LA-UR-05-2657, Los Alamos National Laboratory.)
- T. Asaki, R. Chartrand, C. Powell, K. Vixie, and B. Wohlberg, "Abel Inversion Using Total Variation Regularization," submitted to *Inverse Problems in Science and Engineering*. (Also, a technical report, LA-UR-05-0680, Los Alamos National Laboratory.)

### Talks and Presentations

T. Asaki and R. Chartrand, "Tomographic Methods for Limited View Angles and Sparse Data," Montana State University, invited talk, September 2004. (Also, a technical paper, LA-UR-04-5767, Los Alamos National Laboratory.)

Borozdin, et al., "Information Extraction from Muon Radiography Data," Int. Conf. on Cybernetics and Inf. Tech., Systems and Applications, Orlando, Fla., July 2004.

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- R. Chartrand, et al., "Detecting Nuclear Materials from Muon-Scattering Data," AAAS annual meeting, Washington, D.C., February 2005.

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Schultz, et al., "Image Reconstruction and Material Z Discrimination via Cosmic Ray Muon Radiography," Nuclear Instruments and Methods A 519:3, 687, March 2004. (Also, a technical report, LA-UR-03-4806, Los Alamos National Laboratory.)